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DEVELOPMENT OF PROPERTY MODELS WITH UNCERTAINTY ESTIMATE FOR RELIABLE PRODUCT-PROCESS DESIGN

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Physical and thermodynamic properties of pure components are vital pre-requisites for performing tasks such as, process design, computer aided molecular product design among others. While use of experimentally measured values for the needed properties is desirable, the experimental data for the properties of interest may not be available in many cases. Also, product-process design involving new molecules require property models to be predictive. In such cases, predictive property estimation methods such as group-contribution$^+$ (GC^+) approach are generally suitable to obtain the needed property values. Also, in addition to the accuracy of the property estimates, the design engineer requires to consider uncertainties in the estimated property values in order to assess the quality and reliability of the final design. As a consequence, development of efficient and reliable property prediction methods and tools that can also provide estimates of uncertainties in predictions of properties becomes necessary.

The objective of this work is to develop a systematic methodology to provide more reliable predictions with a new and improved sets of model parameters for GC^+ approach (combined GC models with atom connectivity index (CI) based models) together with the results of uncertainty analysis such as covariance matrix needed to quantify the uncertainties in the estimated property values. In total 21 properties of pure components, which include normal boiling point, critical constants, normal melting point, standard Gibbs energy among others have been modeled and analysed. The statistical analysis of the model performance for these properties is highlighted through several illustrative examples. Important issues related to property modeling such as thermodynamic consistency of the predicted properties (relation of normal boiling point versus critical temperature etc.) have also been analysed. The developed methodology is simple, yet sound and effective and provides not only the estimated property values using the GC^+ approach but also the uncertainties in the estimated property values. This feature allows one to evaluate the effects of these uncertainties on the product-process design calculations thereby contributing to better-informed and reliable engineering solutions.